Cation Ordering in Minerals at High Pressure

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Introduction: Order-disorder phenomena play a key role in the energetics and crystal chemistry of minerals. Variation of cation order-disorder distribution result in changes in free energy, therefore phase stability and physical properties, such as strength, elastic moduli, and thermal conductivity. Study the cation order-disorder phenomena in mantle minerals at high pressure and temperature in important to understand accurately the physical properties of the minerals in the Earth interior. Most of previous studies on cation ordering focus on the temperature dependence. Studies on pressure effect are few, and most of them are carried out by investigating quenched samples. However, as pointed out by many authors[1,2], anomaly in the temperature dependence indicates that cation ordering state is hard to quench from very high temperature because of fast kinetics. Therefore *in situ* measurements are essential to better understand the pressure and temperature effect on cation ordering in minerals.

Methods and Materials: The experiments were performed using the large anvil press SAM85 at the superconductor wiggler Beamline X17B1. Monochromatic x-ray diffraction was collected using a combined CCD/IP system[3] for structure refinements. The materials that have been studied include $MgFeSi_2O_6$ pyroxene, $NiAl_2O_4$ spinel, and MgTi2O5 Karrooite.

Results: $MgFeSi_2O_6$ clinopyroxene is an unquenchable high pressure phase. We have successfully collected high quality diffraction data from this phase. Structure refinements will yield the first result on the Mg/Fe cation ordering in this phase. Decomposition was observed in both $NiAl_2O_4$ spinel and MgTi2O5 Karrooite at high pressure and temperature. Structure refinements will reveal details of cation ordering and structural change before and during the decomposition.

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